Theory and Simulation Issues and Challenges

Peter J. Catto

(with lots of help)

Representing
Theory Coordinating Committee
& Theory Program

March 14, 2007

Motivation: Changing Role of Theory

- **The role of basic plasma theory has changed**
  - **Also need to insure the proper physics is in simulations to make them predictive**
- **Traditional role**
  - **Directly interpret experiments - but in improved operating regimes**
  - **Continue striving for a deeper understanding**
- **Descriptions must be valid for longer times**
  - **MHD time scales no longer adequate**
  - **Drift time scales becoming inadequate**
  - **Ultimately need to simulate on transport time scales**
- **Added role: Basic theory needed to build predictive simulations on transport time scales**

Overview

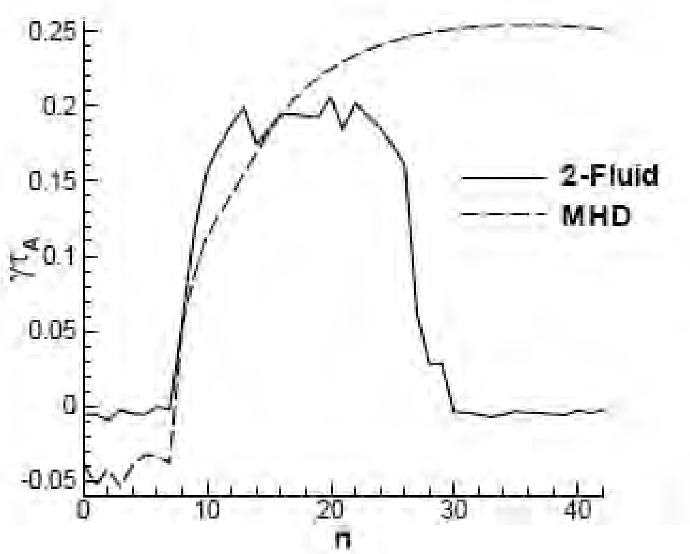
- **Theory status and long range goals**
  - Focus on simulations and physics improvements
  - Physics issues to be addressed and ultimate goals
  - Mix in basic theory applications to experiments
- **Simulation examples - can't cover all theory!**
  - Extended MHD or 2 Fluid
  - RF/CD and Integration
  - Gyrokinetics (including edge)
- **Purple text denotes basic plasma theory input needed to deal with an issue**
- **Concluding remarks**

Extended MHD (X-MHD) or 2 Fluid

- NIMROD and M3D intended to handle
  - reconnection (sawteeth) and resistive effects
  - ballooning and peeling (ELMs)
  - disruptions
  - neoclassical tearing modes (NTMs)
- MHD Problem: ultraviolet catastrophe
  - growth rate increases with n = mode number but codes retain a finite number of n
  - using phenomenological/hyper diffusivities/resistivities
- Basic plasma physics solution
  - add diamagnetic (or FLR) effects

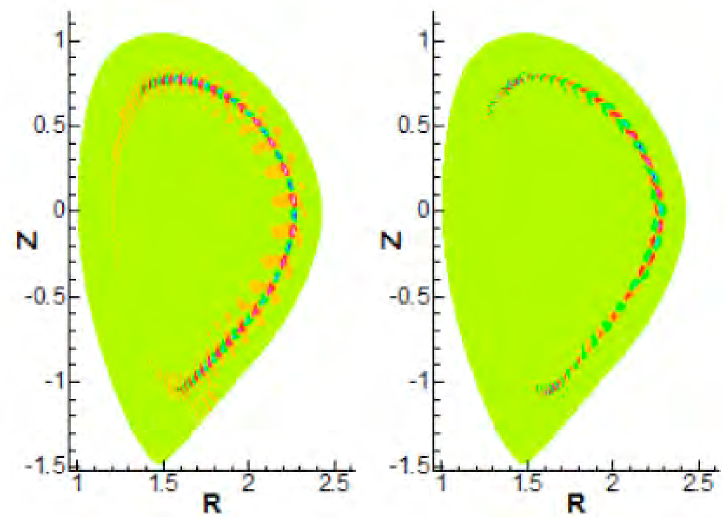
ELM Milestone: NIMROD Linear Results

Linear spectra



Linear eigenfunctions

MHD (n = 21) 2 fluid (n = 21)



2 fluid stabilization of high n modes

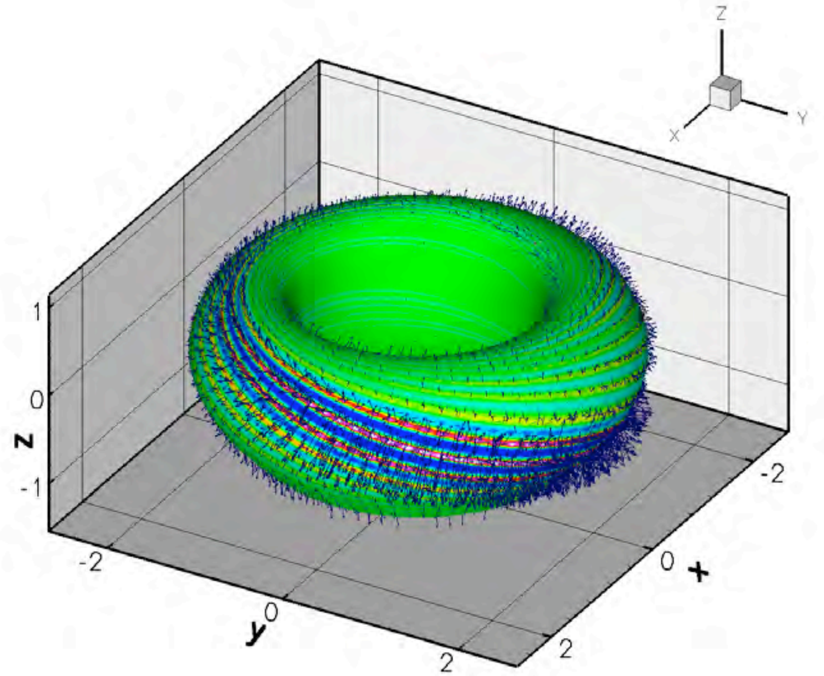
2 fluid eigenfunctions: localized and sheared

(using same radial diffusivities)

ELM Milestone: Nonlinear Results

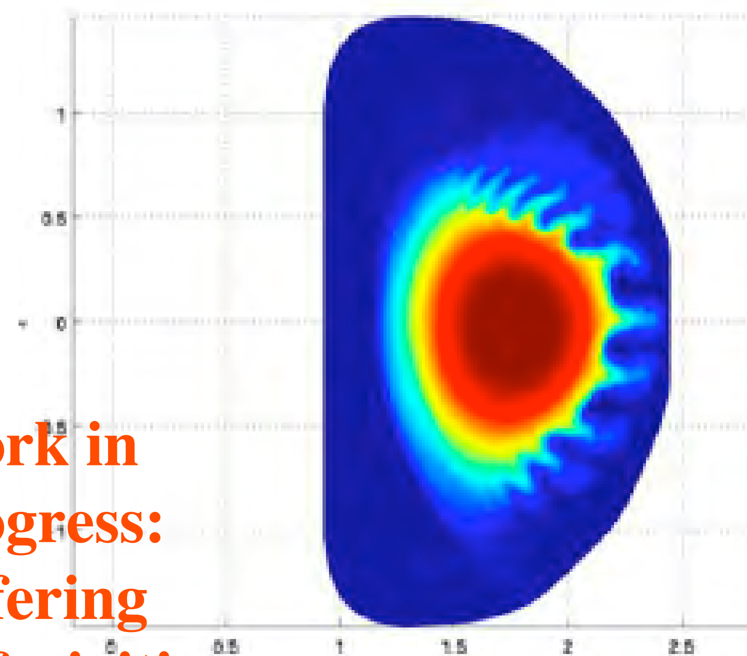
2 fluid gives helically localized mode about q = 3 surface, while MHD has fingers

2 Fluid: helical, localized



Broad range of unstable modes with nearest neighbor coupling

MHD: plasma fingers



Work in progress: differing diffusivities and heat balance models

Fingers broken-up by shear in toroidal flow

Entering a New Era: Diamagnetic Effects

- **Diamagnetic effects are larger than radial transport (also needed) and enter via**
  - diamagnetic heat flux
  - gyroviscosity
  - results must be insensitive to phenomenology
- **Future extensions needed**
  - full drift gyroviscosity instead of Braginskii
  - perpendicular and parallel viscosities
  - f from drift kinetic equation for closure: a biggie! (consistent theory descriptions need to be developed)
  - improved separatrix?
- **Verification possible in some limits**
  - short mean free path limit
  - isothermal limit - a useful test

Isothermal Tokamak Operation

- **Steady state isothermal tokamak**
  - **rigidly toroidally rotating Maxwellians for arbitrary collisionality**
  - **density profile exponential and electrostatic potential linear in poloidal flux**
  - **stress = Reynold's stress** $Mn\mathbf{VV}$ **+ scalar pressure** p **(gyro, parallel & perpendicular viscosities vanish)**
- **Complications due to**
  - **temperature variation**
  - **waves: time variation & departures from axisymmetry**
  - **zonal flow: time varying axisymmetric, driven by waves**

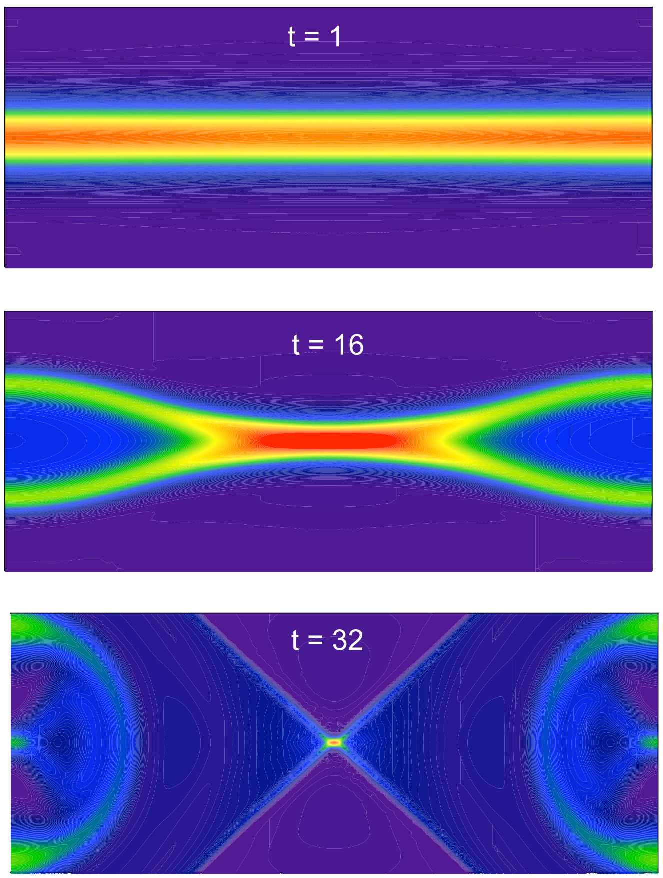
Other X-MHD Results Include:

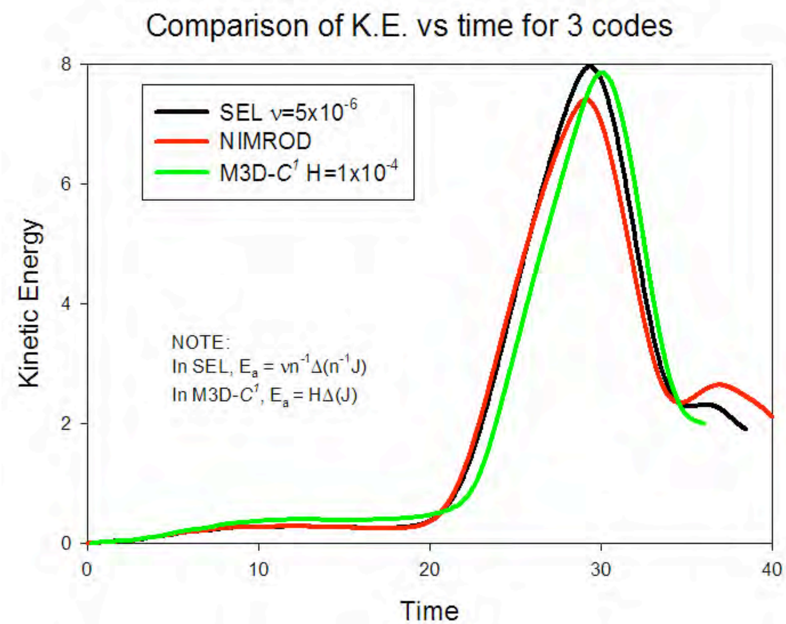
- Braginskii gyroviscosity tests:
  - verified against gravitational mode theory
  - verified theory of magnetothermal instability
  - 2D GEM reconnection modified*
- Gyroviscous cancellation: often too crude!

Some MHD Results

- Resistive MHD sawtooth simulations
  - NIMROD & M3D comparisons underway*
- Gas jet disruption mitigation on C-Mod
- Poloidal flux amplification in SSPX

Current Density Contours for GEM* Nonlinear Benchmark





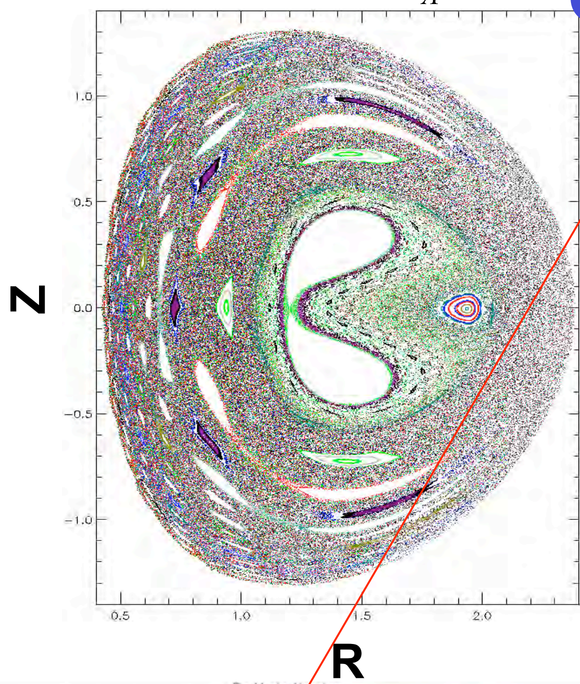
* Geospace Environmental Modeling

- Non-linear reconnection benchmark: 3 codes using full 2-fluid model
- Current density (out of page) for t > 20 collapses due to 2-fluid effects
- Extending to strong guide field for collisionless tokamak reconnection

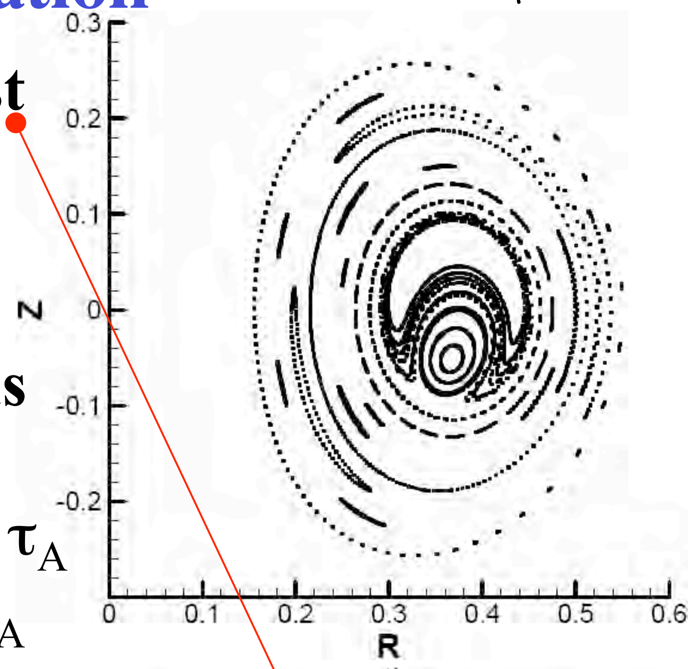
Flux Surfaces at 2nd Sawtooth Crash

CDX-U simulation

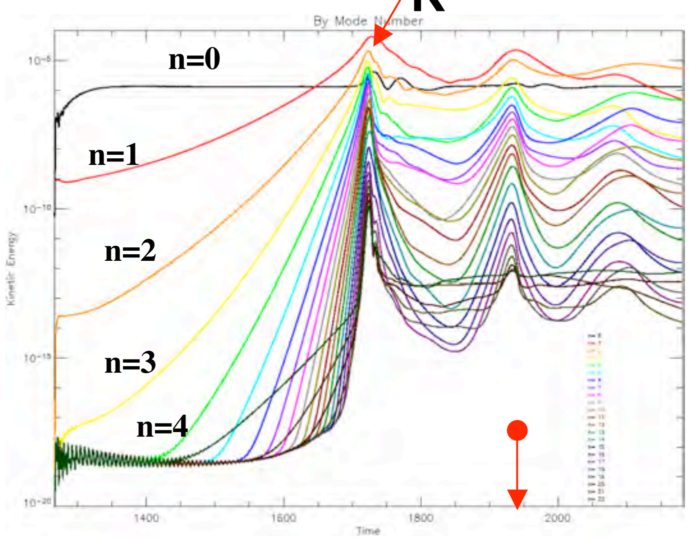
M3D: t = 1936 τ_A

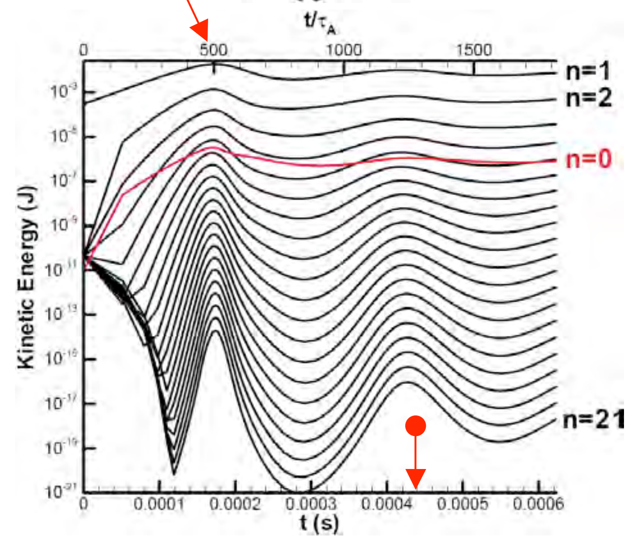


NIMROD: t=433 μs



- **~ 500 τ_A to 1st crash for both** (T loss small)
- **Crash periods differ:** NIMROD~710 τ_A & M3D~ 212 τ_A
- **Crash time faster in M3D**
- **M3D stochastic during crash**





X-MHD: Challenges

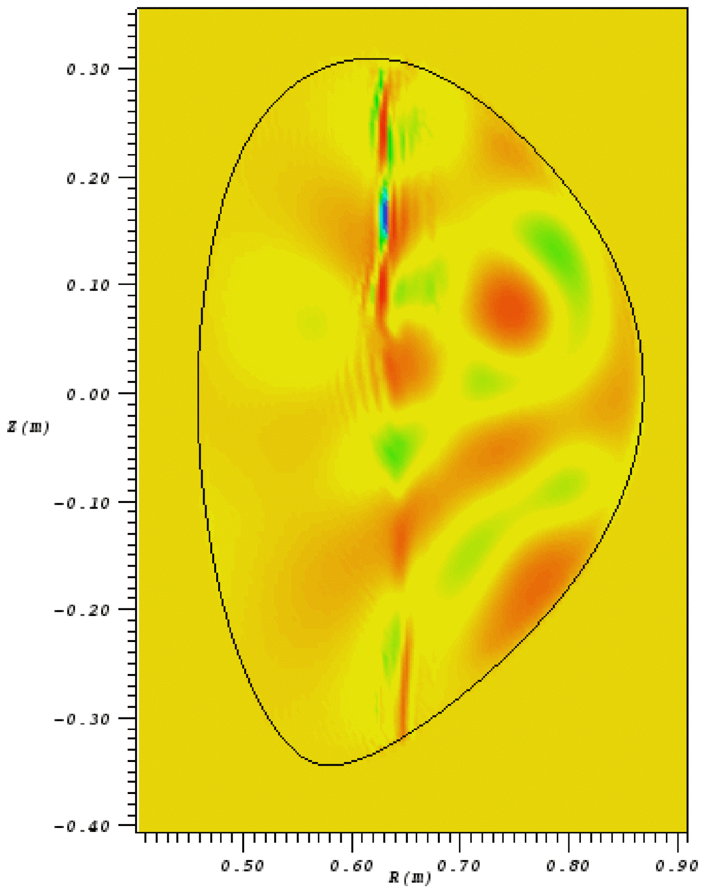
- Determine the nonlinear behavior of ELMs
  - Fingers vs. helix or something else?
- Resolve sawtooth modeling issues
  - Numerics and/or energy balance? Diamagnetics?
- Kinetic suppression of resistive wall mode
- Complete diamagnetic treatment for drift ordering
  - Drift form of gyroviscosity
  - Physical viscosities, resistivities & diffusivities
  - Arbtrary collisionality requires an f
- Couple to a drift kinetic equation to get f
  - Non-trivial, long term and hard!
  - Desire simpliest self-consistent model

RF/CD and Integration

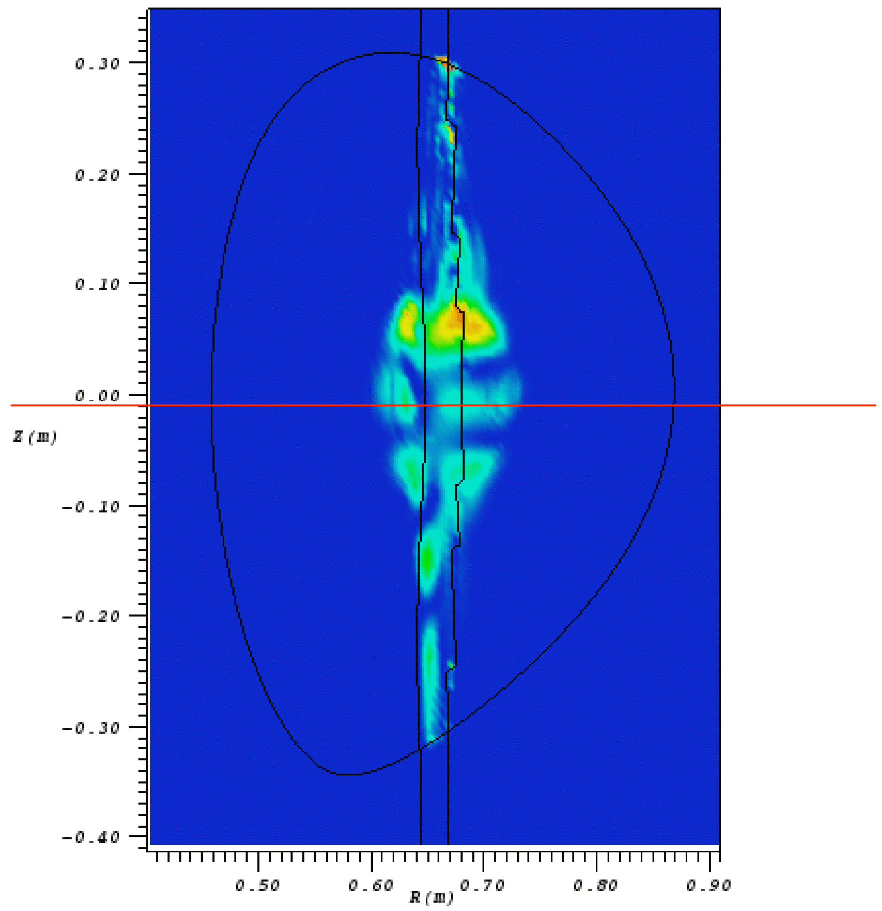
- Wave propagation physics: full wave codes
  - TORIC: faster, but gyroradius < wavelength
  - AORSA: slower, but gyroradius ~ wavelength
- Fokker-Planck + quasilinear kinetic codes
  - CQL3D: 2 velocity + radial (transit averaged)
  - ORBIT-RF: finite radial orbit effects
- Coupled
  - kinetic code provides f for full wave code dielectric
  - full wave code provides fields for quasilinear operator
- Quasilinear validity
- Nonlinear effects in sheaths

AORSA+CQL3D: power deposition contours exhibit asymmetry needed to reproduce energetic ion tail measurements during minority heating on C-Mod

Wave fields



Heating



Reproduces fast ion tail evolution

Quasilinear Validity for ICRH

ORBIT-RF shows large RF electric field destroys superadiabaticity by introducing phase stochasticity

Low fields: waves & particles locked, energy kicks reinforced

High fields: phase coherence and adiabaticity destroyed in a time step

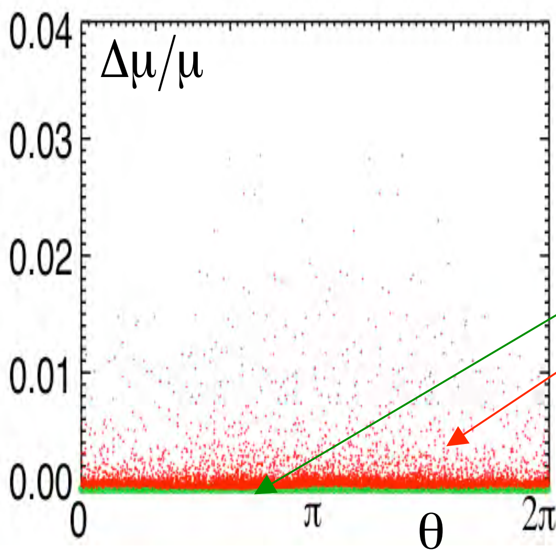
C-Mod minority heating case:

P_{RF} = 0.6 MW

$E_{RF} \approx$ 1 kV/m

ε= 0.428 (mapping parameter)
(stochastic threshold ε = 0.25)

magnetic moment



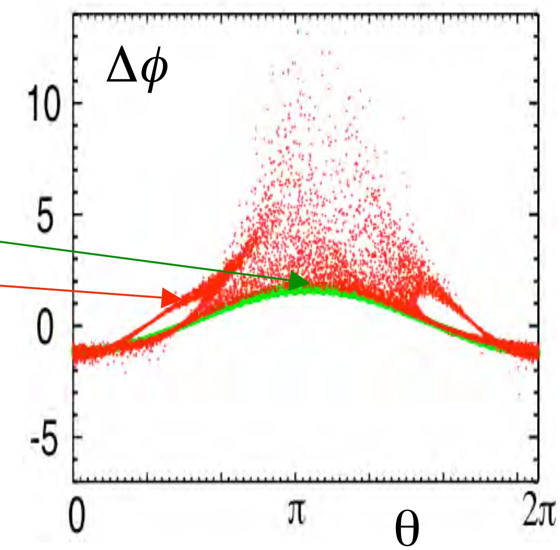
$$\Delta\phi = \frac{1}{2\pi}\int(\omega - \Omega_{ci} - k_{//}v_{//})\frac{ds}{v_{//}}$$

Green = 0.1 kV/m

Red = 1 kV/m

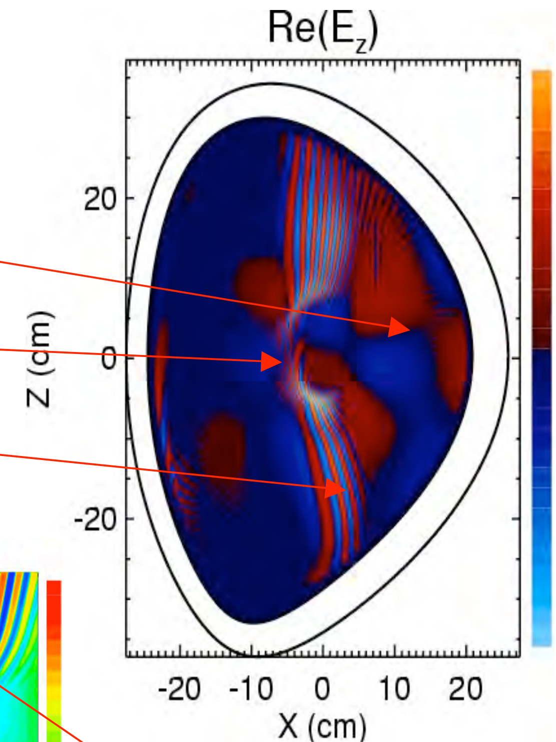
Mechanism works without collisions

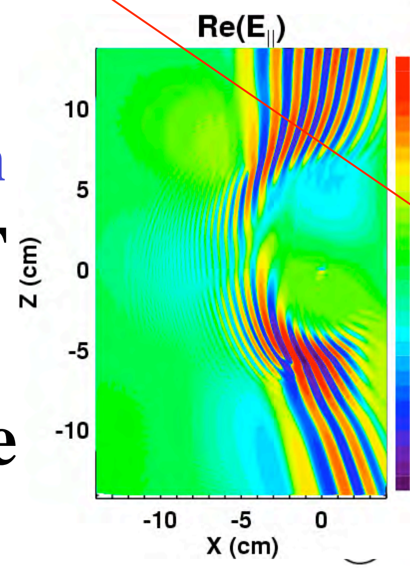
wave phase

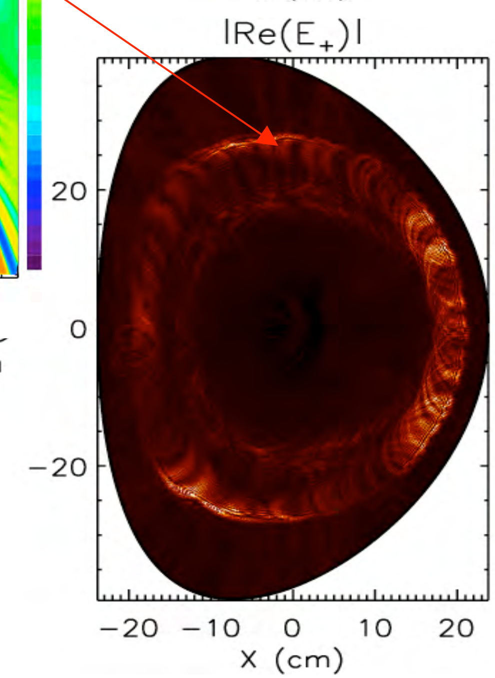


RF/CD and Integration

- **Fast wave mode conversion**
  - ion Bernstein wave
  - Ion cyclotron wave
- **Lower hybrid wave field**
  - similar to ray tracing
  - but includes diffraction
- **CQL3D or ORBIT-RF provide non-thermal f, TORIC will soon provide the quasilinear fields**
- **Plan: 1st studies of LHCD with full wave + FP/QL**

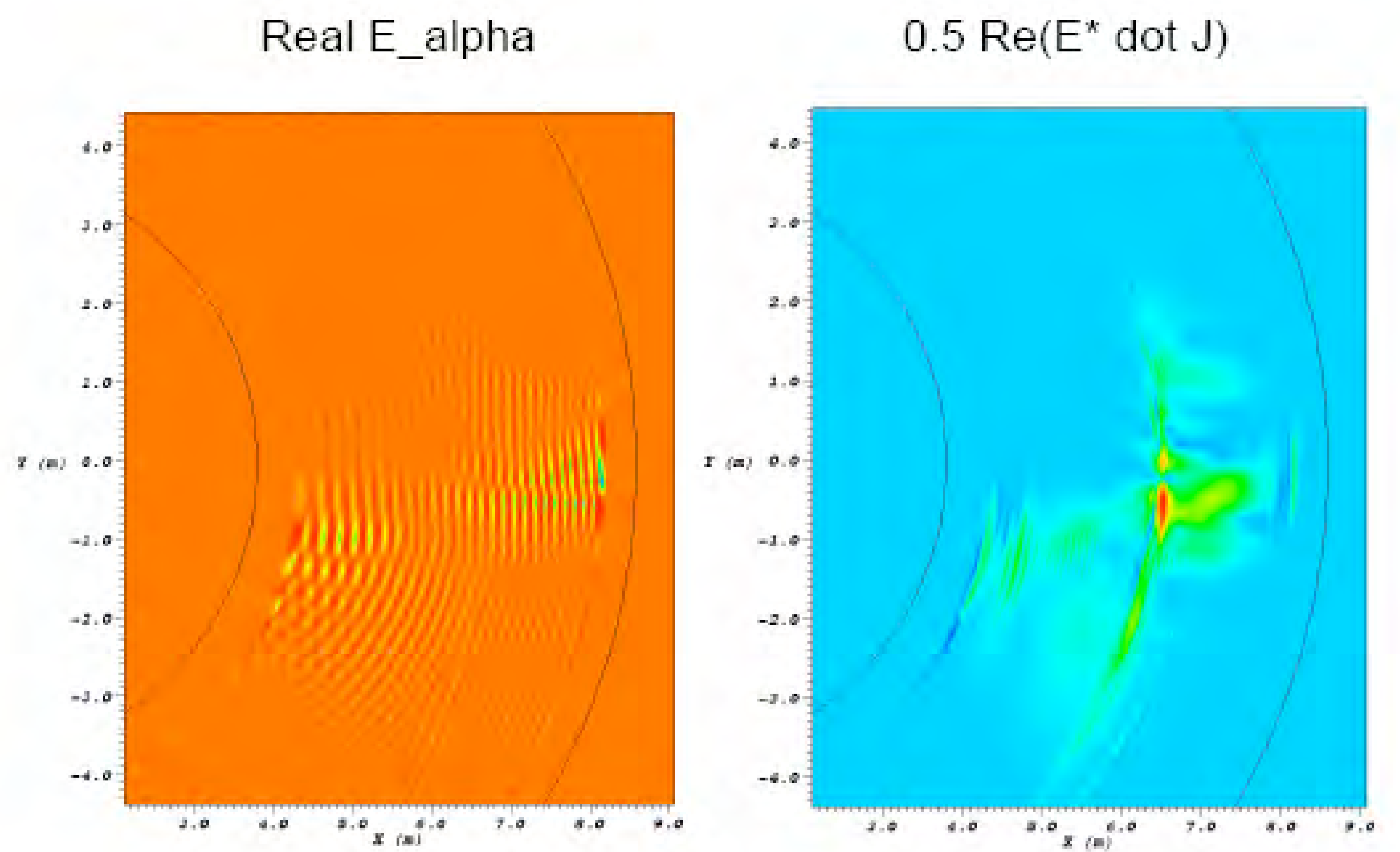






AORSA: FWCD field and power absorption in ITER equatorial plane

(phasing = - π/2 and 169 toroidal modes for finite antenna)

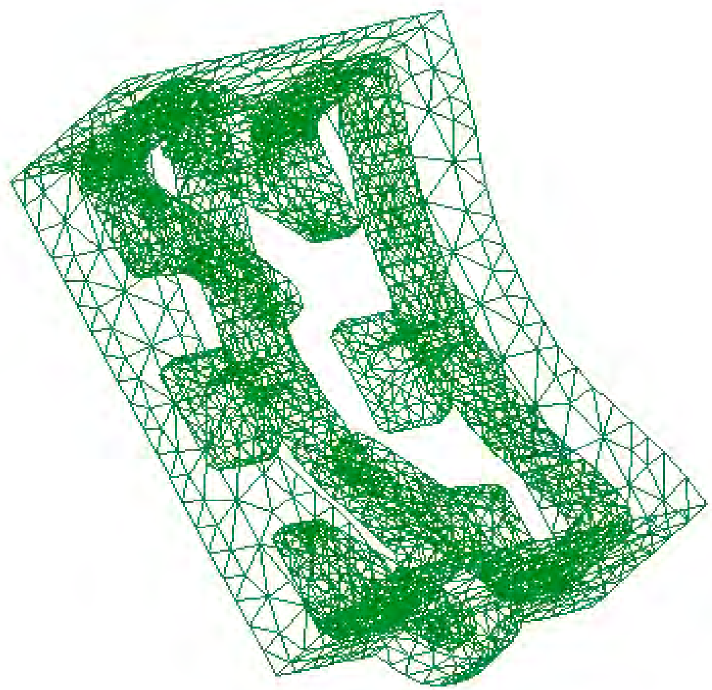


CCW propagation

12/11/2006

ICRF Antenna Modeling:
TOPICA – TORIC Integration

- **TOPICA:**
  - **3D antenna (includes Faraday shield, box,…)**
  - **parallel version to model ITER ICRF antenna**
- **TORIC:**
  - **TOPICA provides fields as a boundary condition for TORIC**
  - **TORIC provides plasma response including effects antenna curvature**



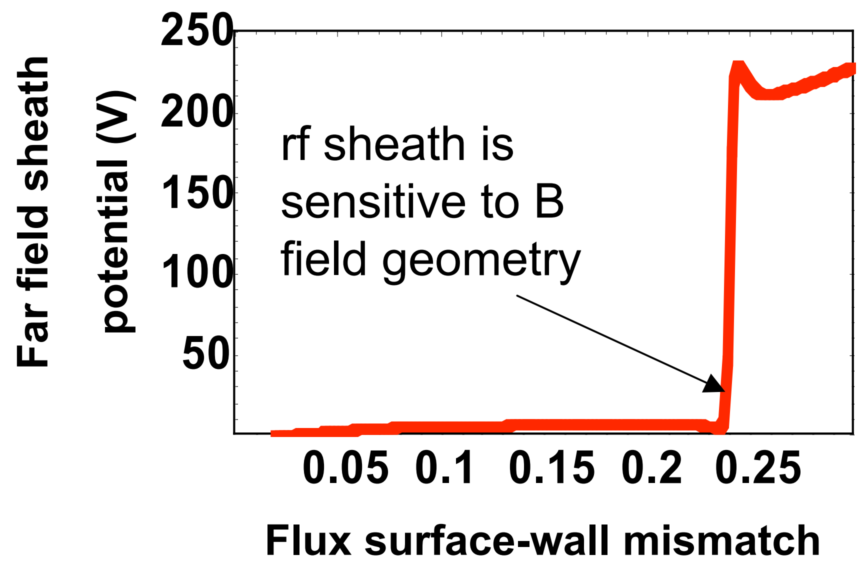
Alcator C-Mod: E antenna

Nonlinear RF Sheath Physics:
modifies TOPICA fields used in TORIC

- **Parasitic effects from antenna and wall sheaths dissipate power by accelerating ions into metal (heating efficiency can drop by 50% or more)**
- **RF fields from TOPICA must be modified**
- **Sheath losses are sensitive to geometry**

Future applications

- **Integrated RF- turbulent transport in SOL**
- **ITER antenna scenario optimization**
- **heating efficiency**



RF/CD Simulations Building on Past Success

- **Full wave and FP+QL codes being integrated**
  - CQL3D & ORBIT-RF provide f to TORIC & AORSA
  - TORIC will provide fields to CQL3D & ORBIT-RF
  - coming soon: first LHCD results from integrated full wave plus FP+QL model with a non-Maxwellian f
- **Antenna modeling being improved**
  - realistic antenna fields from TOPICA for TORIC
  - simulations of nonlinear sheath dissipation begun
- **Integration of TSC and TRANSP**
  - TSC is free boundary code with 1.5D transport
  - TRANSP provides its sources (heating, CD, NBI)

RF/CD Integration: Challenges

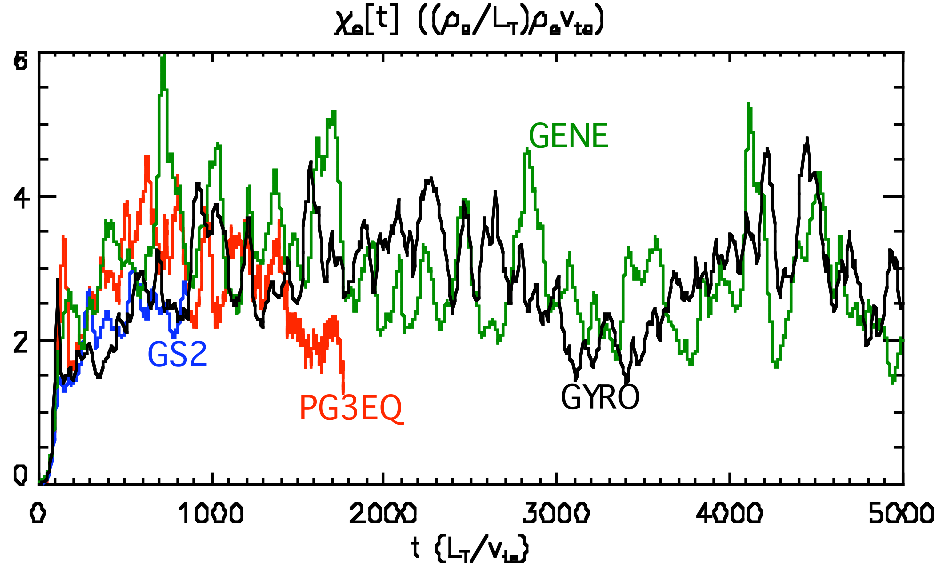
- **Improve treatment of up-down asymmetries**
  - asymmetric part of f can matter
- **Improving and developing nonlinear features**
  - sheath effects
  - stochastic thresholds for various waves
  - wave-particle perturbed orbit interactions
  - parametric instabilities & pondermotive effects
- **Integrate X-MHD, full wave & FP+QL to treat NTMs: many year project!!!**
  - heating & currents from full wave in X-MHD
  - same f for X-MHD and full waves
  - an f from a full drift kinetic equation with FP+QL (coupling of full wave and FP+QL is a start)

Gyrokinetics + Edge

- **Core turbulence modeling**
  - electron temperature gradient (ETG) comparisons
  - trapped electron mode (TEM) results from GS2
  - recent results from GYRO on ion temperature gradient (ITG), TEM and ETG
  - new GTC results indicating ITG dominates in DIII-D, while neoclassical dominates in NSTX
- **Turbulence modeling on the transport time scale**
  - gyrokinetic and Poisson equation
- **Edge turbulence and divertor physics**
  - a start on the pedestal and SOL
  - divertor biasing experiments (not GKs)

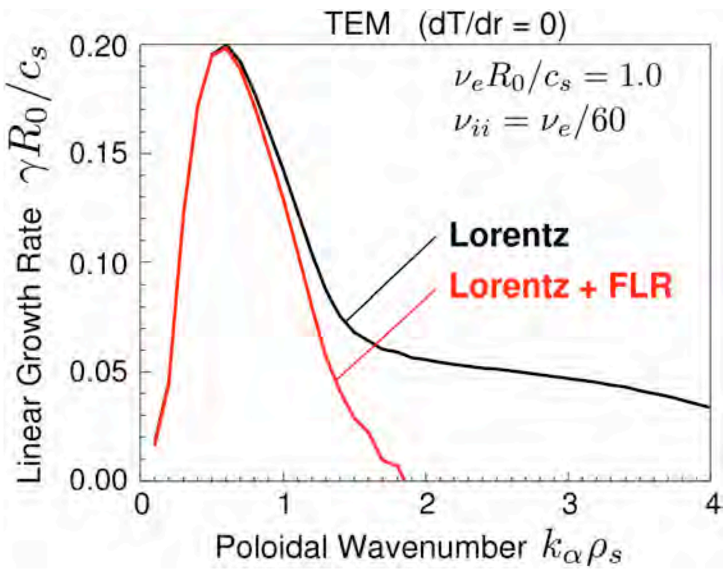
ETG Simulations: convergence tests and code benchmarking put on firm foundation

- **Convergence tests:**
  - excellent convergence in time, velocity space & grid spacing
  - kinetic ions retained
- **Code benchmarking:**
  - excellent agreement between 3 continuum codes (GYRO, GS2, GENE) & 1 PIC code (PG3EQ)
  - working on another PIC code
- **Find:**
  - adiabatic ions fail in high χ_e, high shear regime
  - transport $\chi_e < 15(\rho_e/L_T)\rho_e v_{te}$ is experimentally relevant

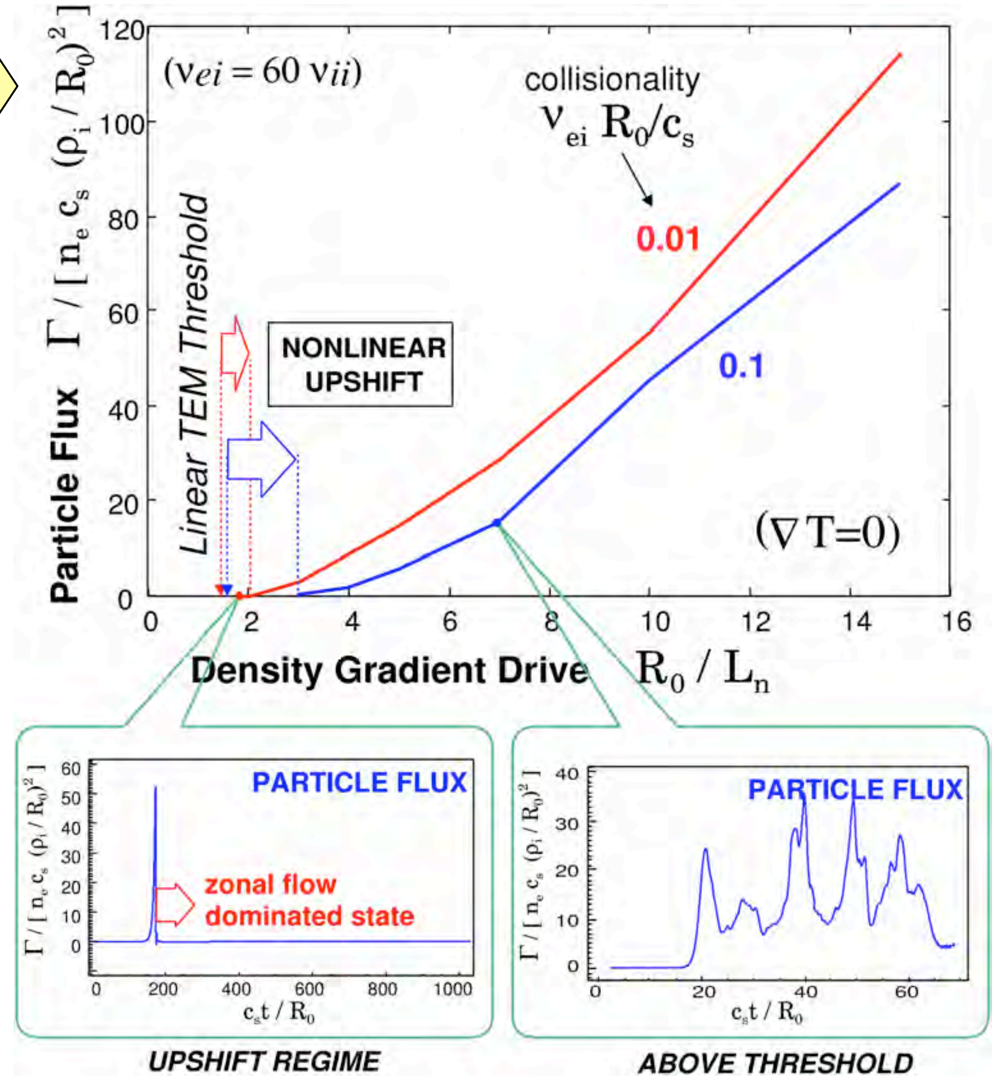


New Collisional Effects on TEM Turbulence: Linear and Nonlinear

Nonlinear upshift of TEM critical density gradient increases with collisionality



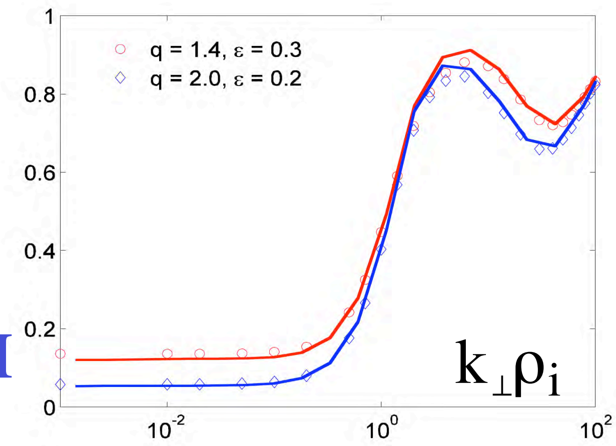
Classical collisional diffusion included in GS2: linearly damps short wavelength TEM



GYRO: Coupled ITG/TEM+ETG Transport

- **Adiabatic ions for ETG inadequate**
  - **transport sometimes unbounded**
  - **problem cured using full ion response**

Zonal flow residual: charge step response



- **ITG transport insensitive to ETG**
  - **ETG secondaries do not affect ITG/TEM**

- **BUT increased ITG drive can reduce ETG transport**
  - **split between linear & nonlinear effects unclear**
  - **ITG/TEM secondary instabilities impact ETG?**
  - **zonal flow generated by ITG/TEM controlling ETG level?**

- **What fraction of χ_e is associated with ETG?**
  - **only 10% to 20% in the absence of ExB shear**
  - **up to 100% if ITG/TEM drive is quenched by ExB shear**

TGLF: a more accurate transport model for integrated modeling

GLF23: predicts tokamak core temperature profiles

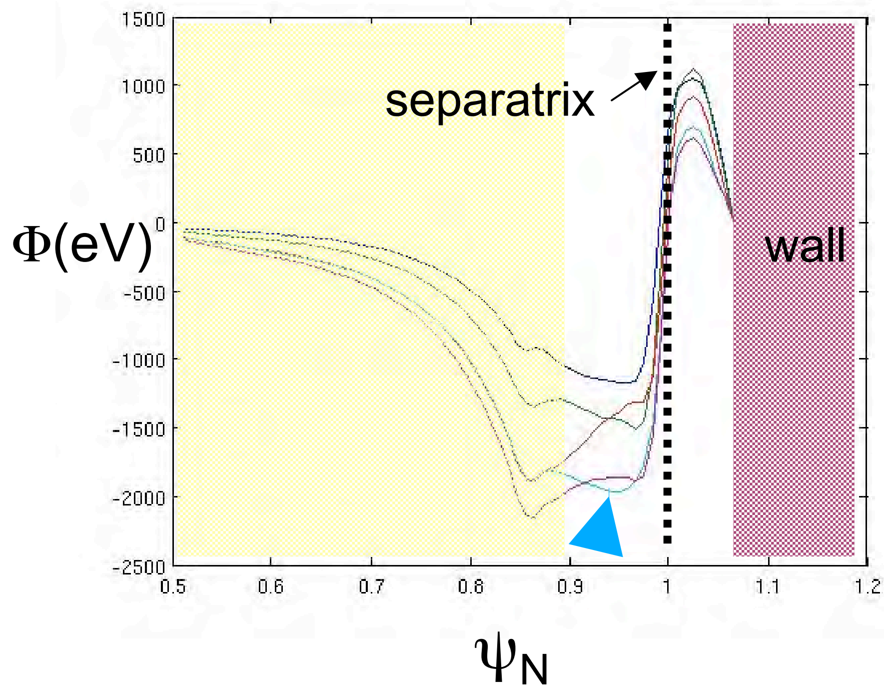
- **TGLF (Trapped Gyro-Landau Fluid): a new transport model using same methodology as GLF23**
  - improves trapped particle treatment compared to GLF23
  - also improves EM, collisional and geometric treatments
- **TGLF: quasilinear transport model better fit to nonlinear gyrokinetic turbulence simulations than GLF23**
- **TGLF: linear stability features used for fast analysis of experiments**
  - growth rates agree with gyrokinetic linear stability codes
  - 100X faster for linear stability analysis of experiments

Practical Gyrokinetic Simulations of Core Turbulence on Transport Time Scales

- **Is there a implementable way to improve the gyrokinetic equation?**
  - GKs arbitrary $k_\perp\rho$ but not arbitrary ρ/L
  - Is a more accurate f needed to evaluate the axisymmetric radial electric field?
  - Does gyroviscosity need to be retained?
- **Is a Poisson equation description adequate?**
  - Is it giving correct axisymmetric radial electric field?
  - Do non-slab magnetic field features matter?
  - Replace by implementable toroidal momentum conservation?
- **Isothermal plasma limit**
  - Do simulations recover a rigidly toroidally rotating Maxwellian as one possible solution?

First Kinetic Solution of Quiescent Edge Plasma from XGC

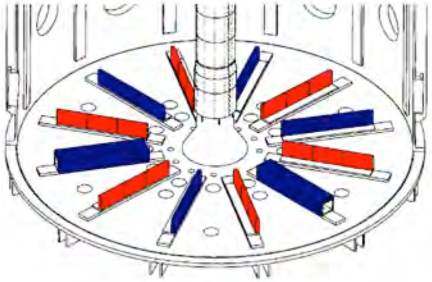
- Edge plasma differs from core: boundary interactions
  - **scrape-off layer**
  - **wall interaction**
  - **ion orbit loss (X-point)**
  - **steep pedestal gradient (~ ρ_{pol})**
  - **non-Maxwellian ions**
  - **neutrals**
- Kinetic simulations necessary
- EM turbulence & M3D/NIMROD coupling: capability being added

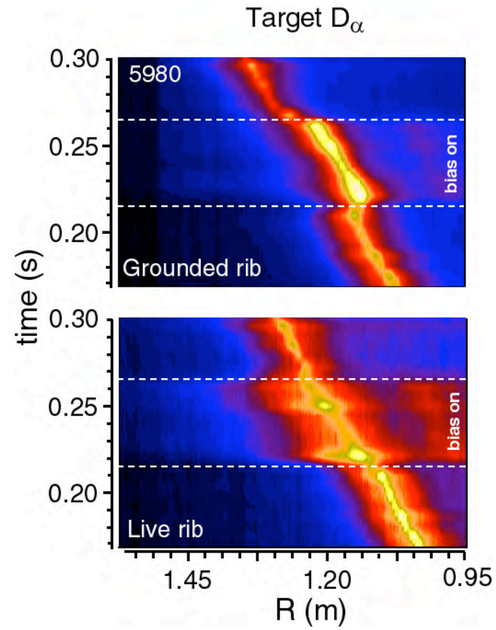


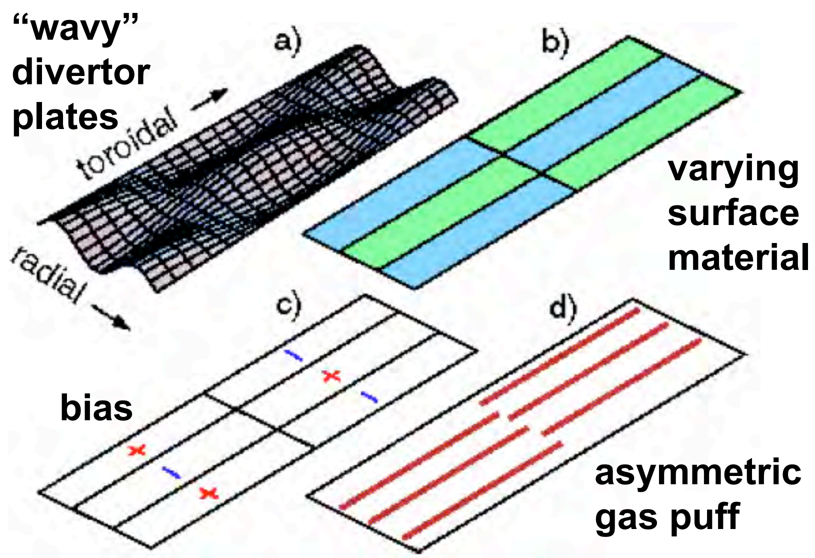
Electric potential of XGC strongly ExB sheared: positive in SOL, negative in pedestal, as in experiments

Theory of Induced Toroidal Asymmetries in Divertor Legs: confirmed on MAST

- **Objective: broaden divertor heat flux**
- **Approach: asymmetric biasing of divertor**
- **Theory: retains sheath boundary conditions & X-point shear**
- **Theory & MAST agree on many biasing effects**
- **Similar experiments planned on NSTX**
- **More reactor friendly approaches (a) & (d) should also be effective**
- **Other topics: multiple X-points & SOL flows**







Gyrokinetics: Challenges

- Improved understanding of ETG
  - What controls the turbulence level?
  - Role of zonal flow on ETG?
- Core turbulence on transport time scales
  - Is there a practical improvement to gyrokinetics?
  - How is the radial electric field determined?
- Edge gyrokinetics: 2 gyrokinetic edge projects
  - Non-Maxwellian gyrokinetics?
  - Treatment of collisions and collisional transport?
  - Isothermal limit recovered? C-Mod SOL flows?
  - Pedestal + separatrix + SOL, neutrals, wall

Theory: Lots of Bang for the Buck!

- ~ $30M/year
- Advanced computing/SciDAC budget (OFES)
  - FY06 (actual): $5,500K
  - FY07 (request): $6,970K
  - FY08 (request): $7,140K
- Basic theory and simulation
  - FY06 (actual): $24,900K
  - FY07 (request): $23,900K
  - FY08 (request): $24,552K
- Maintain a balance between simulations and basic theory - resist robbing Peter to pay Paul
- Avoid “eating our young” by making room for our best and brightest young theorists

A Strong Basic Theory Effort Provides

- Best possible physics support of experiments
  - deeper understanding of theory leads to new ideas and discards bad ideas
  - suggests fresh ways of understanding results
- Highest quality physics to incorporate in predictive simulations
  - desire codes that simulate multiple machines
  - want to go beyond fudge factors or phenomenology
  - ultimately need to model on transport time scales
- Training in basic theory and simulations
  - next generation of theorists must understand what is or needs to be in the simulations they run or build

Issue: Student Training

- Different with SciDACs/FSPs
  - PhD commitment is 5-6 years
  - SciDAC/FSP lasts 3-5 years
  - Risk: accept a student in hopes of getting $, or win $ then find a student who may not have time to finish
  - If a exceptional student appears after 2 years do you accept him or her?
  - Training normally best for theory simulators; often more compatible with a national laboratory setting
- Basic theory support of students
  - Focus is on a deeper understanding of basic plasma theory rather than computational physics
  - More compatible with university setting
- Balance needs of basic theory and simulation

Issue: SciDAC/FSP

- **SciDACs/FSPs**
  - Good: $ & 3-5 years enough time to do something, partnering with computer science & applied math
  - Bad: scientists supported by multiple sources, continuity, more meetings & conference calls
  - Ugly: student training
  - Awkward: proposal writing & reviewing, managing
- **Can we enhance the strengths of these programs and maintain a balance with basic theory?**

Final Thoughts

- What we have learned recently is impressive
  - Simulations have made much of this possible
  - But much more basic theory needs to be done to insure predictability
  - Plasma simulators and theorists must work together to reach this goal
- Key challenges for theorists & simulators
  - Coupling a drift kinetic code to X-MHD (closure issues) and RF/CD simulations
  - Gyrokinetic turbulence on transport time scale and evaluating and understanding the electric field
  - Turbulence simulations in the pedestal and SOL

Predictive Code Development is a Partnership